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# The von Neumann-Wigner type potentials and the wave functions' asymptotics for the discrete levels in continuum

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**Abstract**

One to one correspondence between the decay law of the von Neumann-Wigner type potentials and the asymptotic behaviour of the wave functions representing bound states in the continuum is established.

Many years ago von Neumann and Wigner [1] discovered a class of potentials that gives isolated quantum mechanival levels embedded in continuum of positive energy states. The underlying strategy of these authors was employed in [2] to produce more examples. The main feature of these potentials is oscillations at the spatial infinity together with a relatively slow decrease. A lot of authors have contributed to the sound mathematical substantiation of this extraordinary phenomenon and most of their results are collected in the excellent books of M. Reed and B. Simon [3]. Recently the interest in this problem was excited anew due to its various applications in physics of atoms and molecules. In spite of rather wide publications, as it was noted in

the recent review [4], "there is not as yet a fully systematic approach". In [4] the isospectral technique is applied to generate such kind of potentials.

One of the most fundamental conclusions of all previous investigations is that for so called modulating functions constructed or used there, the normalizable (square integrable) wave functions have only a power-like decay at large distances while potentials vanish in the same limit. Hence, these wave functions can hardly be called bound states in the usual sense, because in general they do not guarantee finiteness even of the square radius of the state.

Below we present a slightly modified, but by our opinion more convenient method that allows to observe one to one correspondence between the decay law of potentials and that of wave functions corresponding to the bound states in continuum. Moreover we will demonstrate that there exist potentials, which lead to wave functions with more rapid than the power-like decrease.

We confine ourselves to considering of S-waves only. Corresponding Schrödinger equation for radial function $\chi$ has the form

$$\chi''(r) + \frac{2m}{\hbar^2}\left[E - U(r)\right]\chi(r) = 0. \tag{1}$$

Denoting

$$\frac{2mE}{\hbar^2} = k^2, \qquad \frac{2mU(r)}{\hbar^2} = V(r) \tag{2}$$

we find from eq.(1) that

$$V(r) = k^2 + \frac{\chi''}{\chi}. \tag{3}$$

Now, following [1][2] we take

$$\chi(r) = \chi_0(r) f(r), \tag{4}$$

where $\chi_0(r)$ is solution of some solvable Schrödinger equation and $f(r)$ is a modulating function. As a rule the free or Coulomb solutions are used for $\chi_0$ [1][2][4] and the boundary condition at the origin $\chi(0) = 0$ is satisfied by a suitable choice of them. As an example let us take the free solution:

$$\chi_0(r) = \frac{1}{k} sin(kr). \tag{5}$$

After substituting (4)–(5) into eq.(3) one obtains [2]

$$V(r) = \frac{f''}{f} + 2k\frac{f'}{f} ctg(kr). \tag{6}$$

We must choose the function $f(r)$ in a manner to provide cancellation of poles of $ctg(kr)$, i.e. the zeroes of $sin(kr)$. Usually it is achieved by taking $f(r)$ to be differentiable function of the variable [1][2]:

$$s(r) = k\int_0^r sin^2(kr')dr' = \frac{1}{2}kr - \frac{1}{4}sin(2kr). \tag{7}$$

Instead of setting the function $f(r)$, we will set its logarithmic derivative

$$\mathcal{C}(r) \equiv \frac{f'}{f}. \tag{8}$$

Then

$$V(r) = \mathcal{C}^2(r) + \mathcal{C}'(r) + 2kctg(kr)\mathcal{C}(r) \tag{9}$$

and the modulating function $f(r)$ can be constructed by solving eq.(8):

$$f(r) = Aexp\left\{\int_0^r \mathcal{C}(z)dz\right\}. \tag{10}$$

First of all we must take care for the above mentioned cancellation of the poles. We can take

$$\mathcal{C}(r) = \phi(r) sin^2(kr). \tag{11}$$

Then the potential becomes

$$V(r) = \phi^2(r) sin^4(kr) + \phi'(r) sin^2(kr) + 2k\phi(r) sin(2kr). \tag{12}$$

Next, to obtain potential that vanishes at the spatial infinity we probe

$$\phi(r) = \frac{a}{r^\beta}, \qquad a = const, \qquad \beta > 0. \tag{13}$$

So the potential takes the form

$$V(r) = \frac{a^2 sin^4(kr)}{r^{2\beta}} - \frac{a\beta sin^2(kr)}{r^{1+\beta}} + \frac{2ak sin(2kr)}{r^\beta} \tag{14}$$

and the corresponding modulating function is

$$f(r) = A exp\left\{ a \int_0^r \frac{sin^2(kz)}{z^\beta} dz \right\}. \tag{15}$$

Evidently, if $\beta > 0$ the last term will dominate in (14) as $r \to \infty$. According to the theorem $XIII.58$ from [3] there are no normalizable wave functions for positive eigenvalues if $\beta > 1$. Validity of this theorem in our case can be checked immediately by studying asymptotic behaviour of (15). Therefore only $\beta \leq 1$ case is of interest. Let us take $\beta = 1 - \epsilon$ with $\epsilon > 0$ ($\epsilon = 0$ case must be considered separately). We have

$$\int_0^r \frac{sin^2(kz)}{z^\beta} dz = \frac{r^\epsilon}{2\epsilon} - \frac{1}{4}\left[\frac{\gamma(\epsilon, 2ir)}{(2i)^\epsilon} + \frac{\gamma(\epsilon, -2ir)}{(-2i)^\epsilon}\right]. \tag{16}$$

Here $\gamma(a, x)$ denotes the incomplete gamma function [5], which has convergent series in positive powers of $x$

$$\gamma(a, x) = e^{-x} \sum_{n=0}^{\infty} \frac{x^{a+n}}{(a)_{n+1}} \tag{17}$$

and the asymptotic expansion in inverse powers of $x$

$$\gamma(a,x) = \Gamma(a) + x^{a-1}e^{-x}\left[\sum_{m=0}^{M-1}\frac{(1-a)_m}{(-x)^m} + O\left(\mid x\mid^{-M}\right)\right]. \qquad (18)$$

It follows that in the limit $r \gg 1$

$$\gamma(\epsilon, 2ir) \approx \Gamma(\epsilon) - (2ir)^{\epsilon-1}e^{-2ir} + O\left(r^{\epsilon-2}\right). \qquad (19)$$

Therefore

$$\int_0^r \frac{sin^2(kz)}{z^{1-\epsilon}}dz \approx \frac{r^\epsilon}{2\epsilon}, \qquad r \gg 1 \qquad (20)$$

and if we take coefficient $a$ in (15) to be negative, then $f(r)$ would have quasi-exponentially decreasing asymptotics leading to square integrable wave functions. Moreover, according to (17) the modulating function $f(r)$ tends to constant as $r$ approaches origin and does not destroy correct boundary behaviour of the wave function $\chi$.

Collecting all above results together we conclude that if the potential has the dominating asymptotics like

$$V(r) \sim -\frac{2\mid a\mid k}{r^\beta}sin(2kr), \qquad 0 < \beta < 1 \qquad (21)$$

then the wave function $\chi$ behaves like

$$\chi(r) \sim sin(kr)exp\left\{-\frac{\mid a\mid r^{1-\beta}}{2(1-\beta)}\right\}, \qquad r \gg 1 \qquad (22)$$

and so decreases fast enough to be normalizable.

Let us consider now the limiting case $\beta = 1$ and define

$$I = \lim_{\sigma\to 0}\int_\sigma^r \frac{sin^2(kz)}{z}dz = \frac{1}{2}\left(ln(kr) - Ci(2kr) + \gamma + ln2\right), \qquad (23)$$

where $\gamma$ is the Euler constant and $Ci(u)$ — the integral cosine, which has the following asymptotics [5]

$$\begin{aligned} Ci(u) &\approx \gamma + ln(u) - \frac{u^2}{4} + O\left(u^4\right) \qquad u \ll 1 \\ Ci(u) &\approx sin(u) + O\left(u^{-1}\right) \qquad u \gg 1 \end{aligned} \tag{24}$$

Therefore

$$\begin{aligned} I &\longrightarrow \frac{1}{2}(kr)^2, \qquad kr \ll 1 \\ I &\longrightarrow \frac{1}{2}ln(kr), \qquad kr \gg 1 \end{aligned} \tag{25}$$

Making use of (24)–(25) in (23) and then in (15), we see that

$$\begin{aligned} f(r) &\longrightarrow const, \qquad kr \ll 1 \\ f(r) &\longrightarrow (kr)^{a/2}, \qquad kr \gg 1 \end{aligned} \tag{26}$$

and therefore

$$\chi(r) \longrightarrow r^{-|a|/2} sin(kr), \qquad\qquad kr \gg 1 \tag{27}$$

It unifies correctly all known results derived for the $r^{-1}sin(2kr)$ asymptotic behaviour of the potential and agrees with the Atkinson's theorem [3].

As a conclusion we can say that there is one to one correspondence between the asymptotic behaviour of potentials decreasing with oscillations and that of wave functions belonging to bound states in continuum. A slight modification of point of view (see eqs.(8)–(12)) allowed us to yield generalized von Neumann-Wigner type potentials with the arbitrary powers of decrease, $\beta \neq 1$. Only $\beta \leq 1$ gives bound states in continuum. Of course the correspondence found above between the asymptotics does not depend on the

method of construction — it is general because its validity depends only on the asymptotic behaviour of the potential under consideration. The last comment we want to make is that the pure exponential decrease $exp(-|a|r/2)$ of the wave function corresponds to potentials that do not vanish at the infinity, but only oscillate (the case $\beta = 0$). The finiteness of any characteristic dimensions of the bound state (like square radius or any higher moments of $r$) makes principal difference between the found new solutions (for $\beta \neq 1$) and the known ones ($\beta = 1$), namely the former are localized like ordinary bound states, while the latter are not.

## References


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